

*spectra*factory

*jan*cami *andrew*markwick-kemper

***A dynamic database of
molecular model spectra***

<http://www.spectrafactory.net>

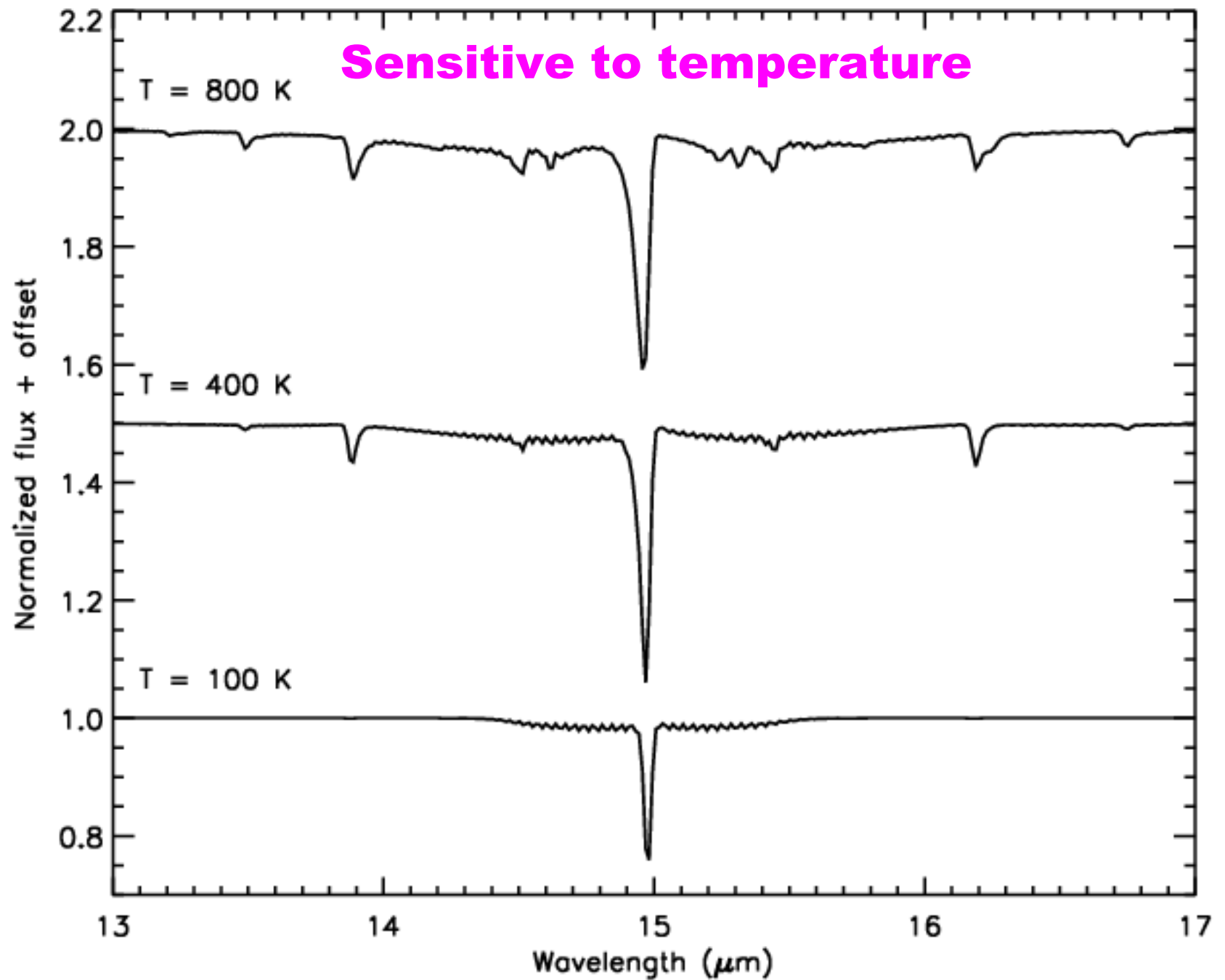
Outline

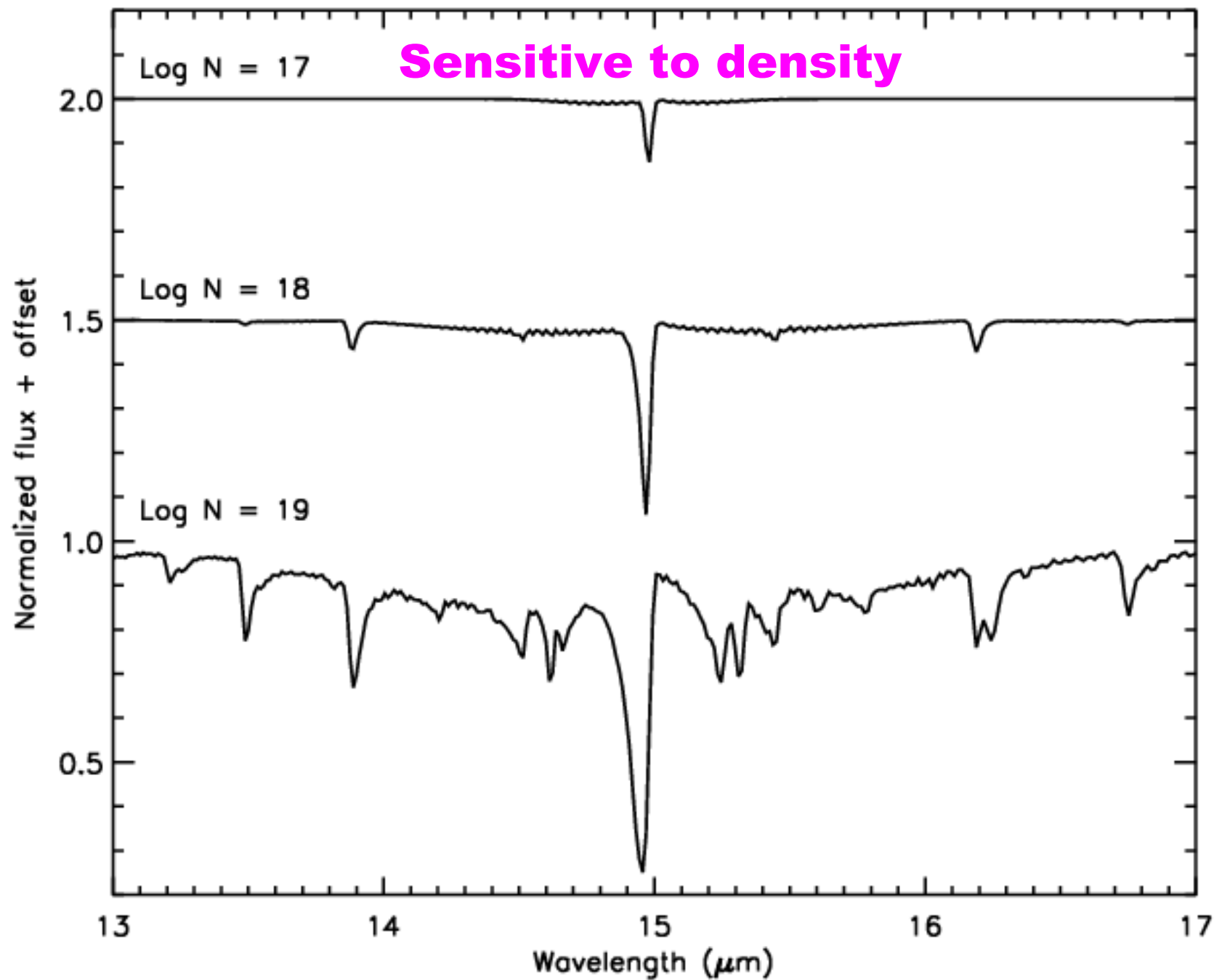
- **Motivation / introduction**
- **The model calculations**
- **The web interface**
- **Current status**
- **Some examples**
- **Future prospects & needs**

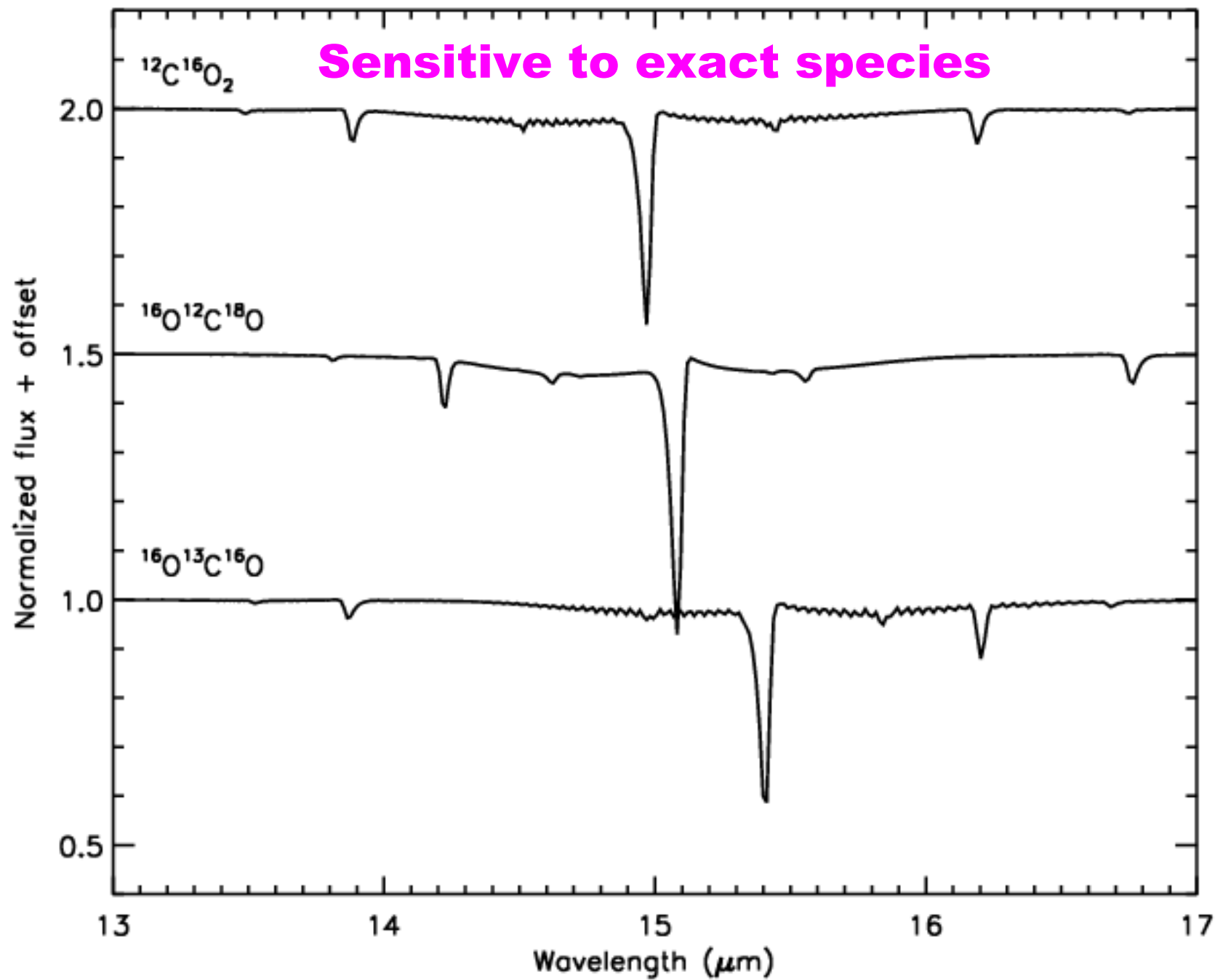
Motivation

- We live in a **molecular universe !**
molecules detected in/around young stars, old stars, interstellar medium, planetary atmospheres, comets, entire galaxies, ...
- Molecules are observed **from UV to sub-mm** wavelengths
- Important diagnostic **tools** & probes !!

Sensitive to temperature







Extracting physical parameters

Identification of species

- Where to find frequencies & line strengths ?**
- Which one of those millions of molecules ?**
- What band profile ?**

Spectral dependence on physical parameters

- Some knowledge of molecular spectroscopy**
- Some knowledge of radiative transfer**

Model fit

- All of the above, plus some statistics**

In an ideal world...

Observed Spectrum



Black box



Perfect Fit



**Physical/chemical
parameters**

Our aim

Observed Spectrum



Grey box



**Best Fit
given limitations**



**Estimate of
Physical/chemical
parameters**

Black box

All possible molecular species

All possible transitions

Full non-LTE radiative transfer

Various geometries

All possible instruments

Robust statistics, fast

Grey box

What's available

What's available

Isotherm, LTE

Slab

On request

Future

Molecular species

143 molecules detected in space

212 including isotopologues

most in sub-mm

42 molecules studied in earth atmosphere

line lists available at 296 K (HITRAN)

often infrared

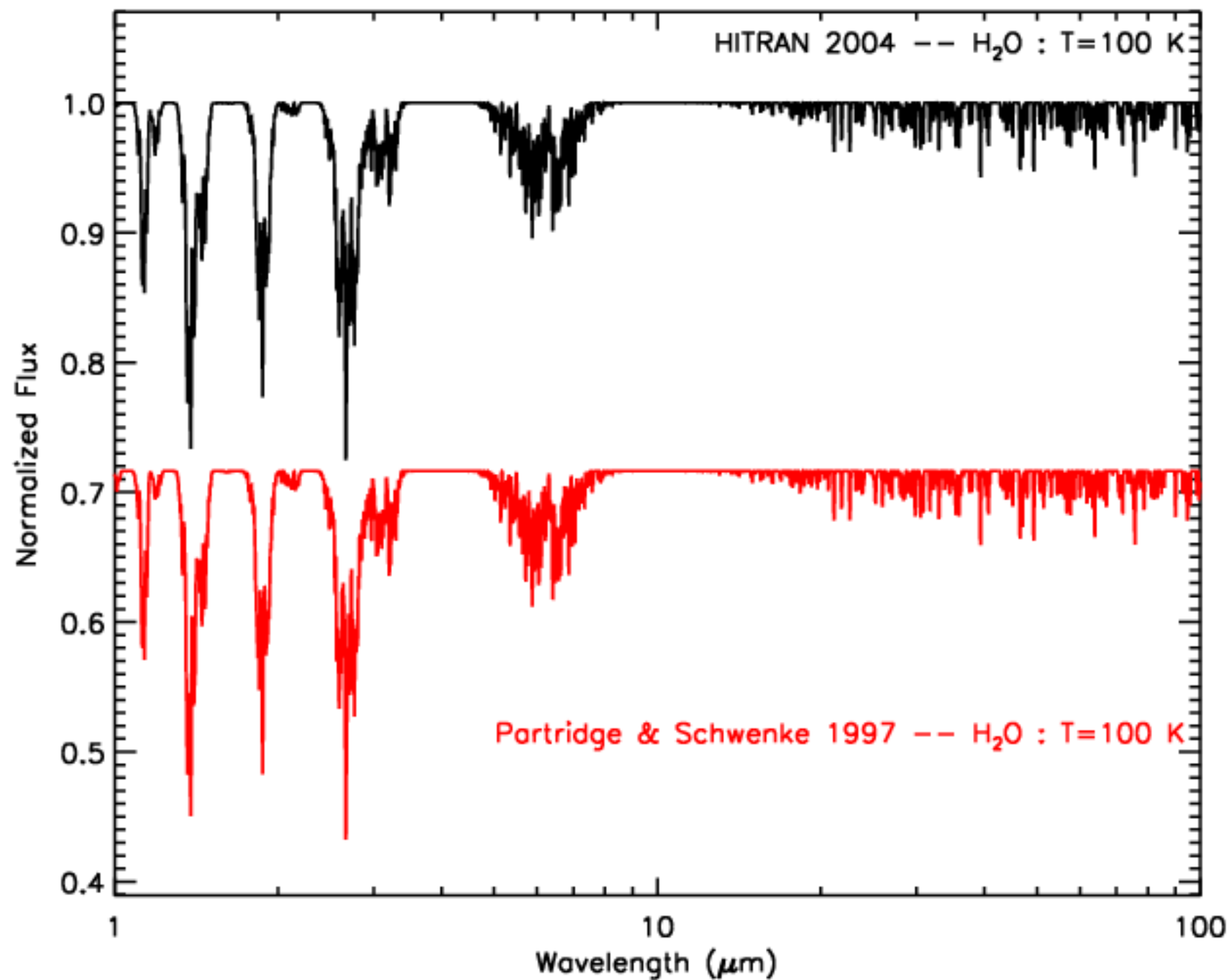
5 molecules with good line lists

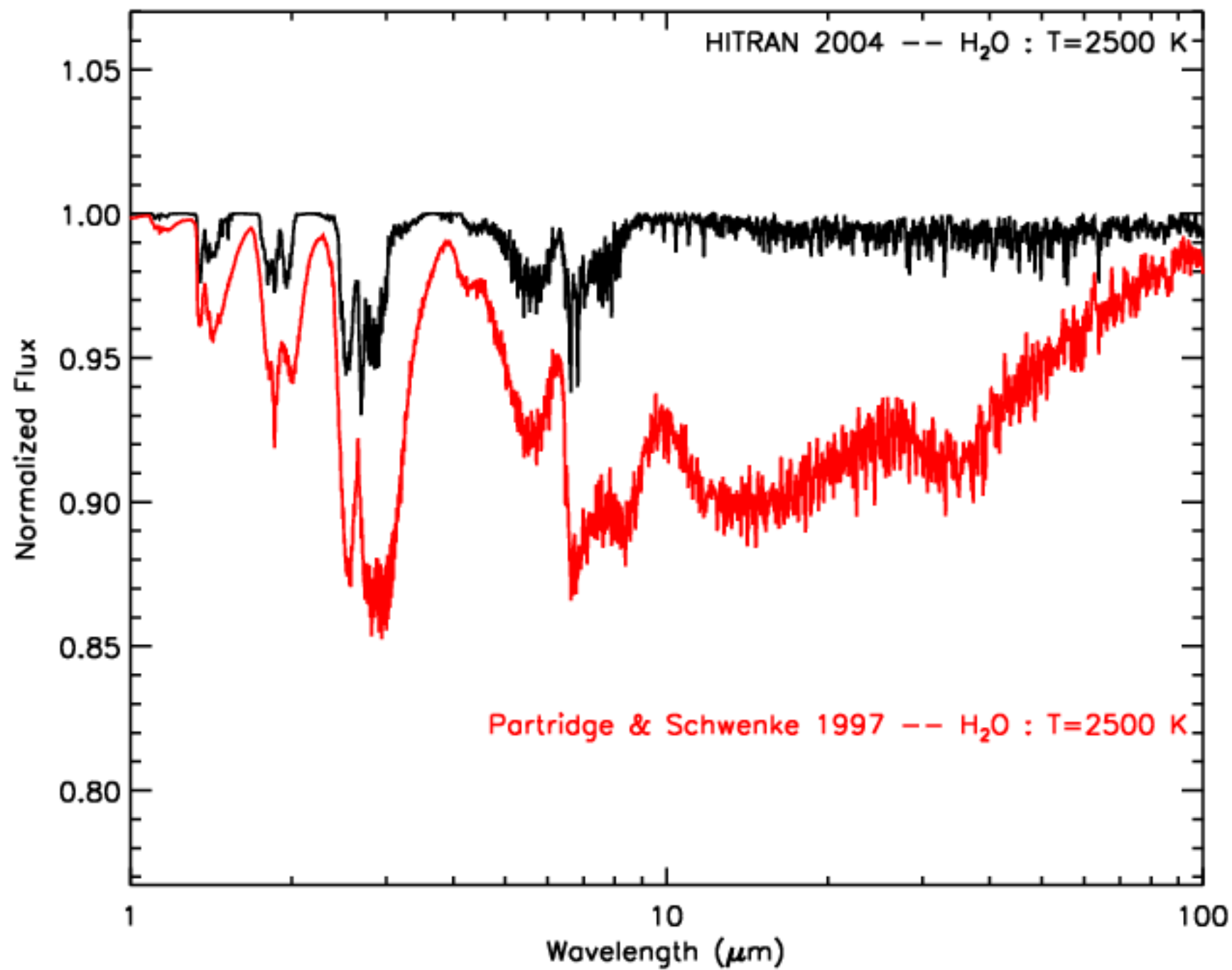
H₂O, TiO, SiO, CO, CO₂

Large frequency range

Many levels (electronic, vibrational, rotational)

High temperatures



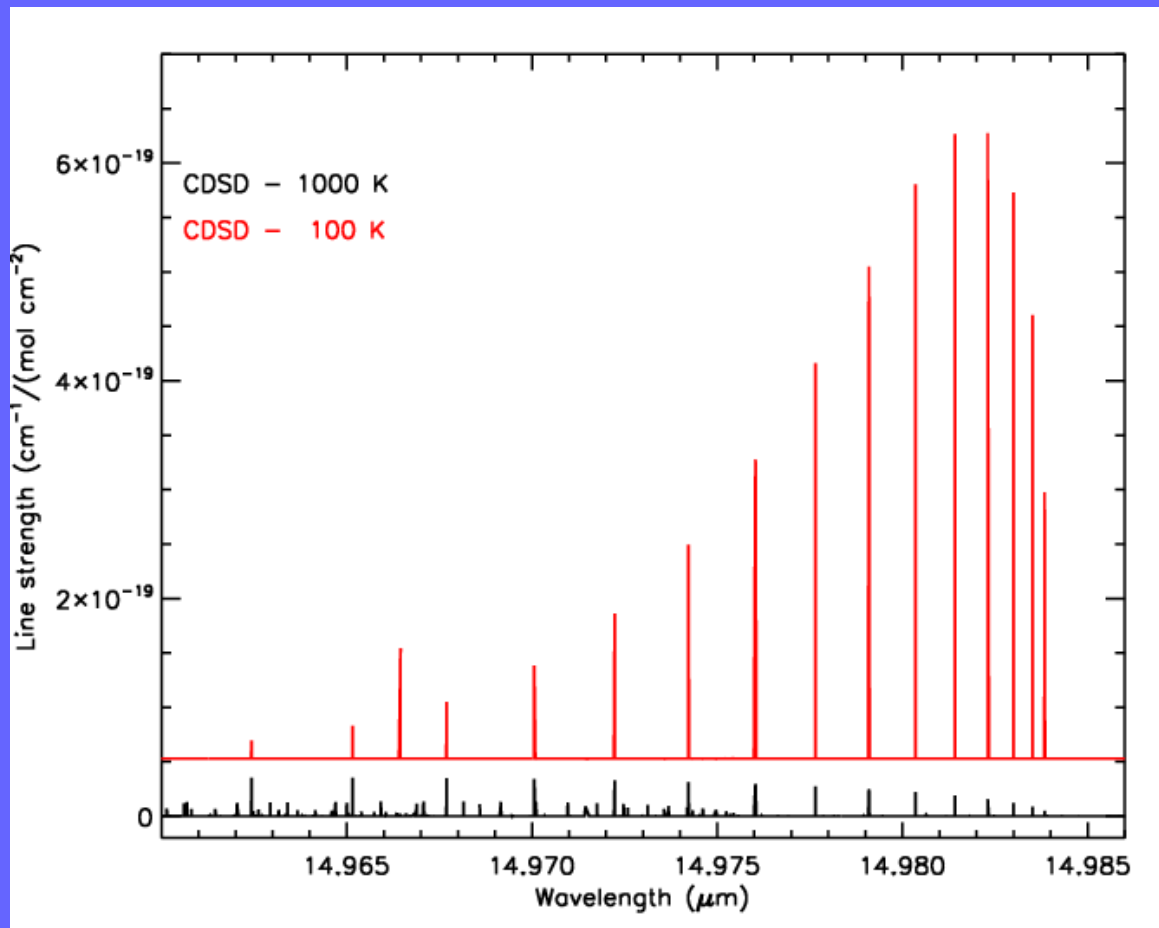


Model calculations I

Line list : Frequencies of transition

Intrinsic line strength at T_{ref}

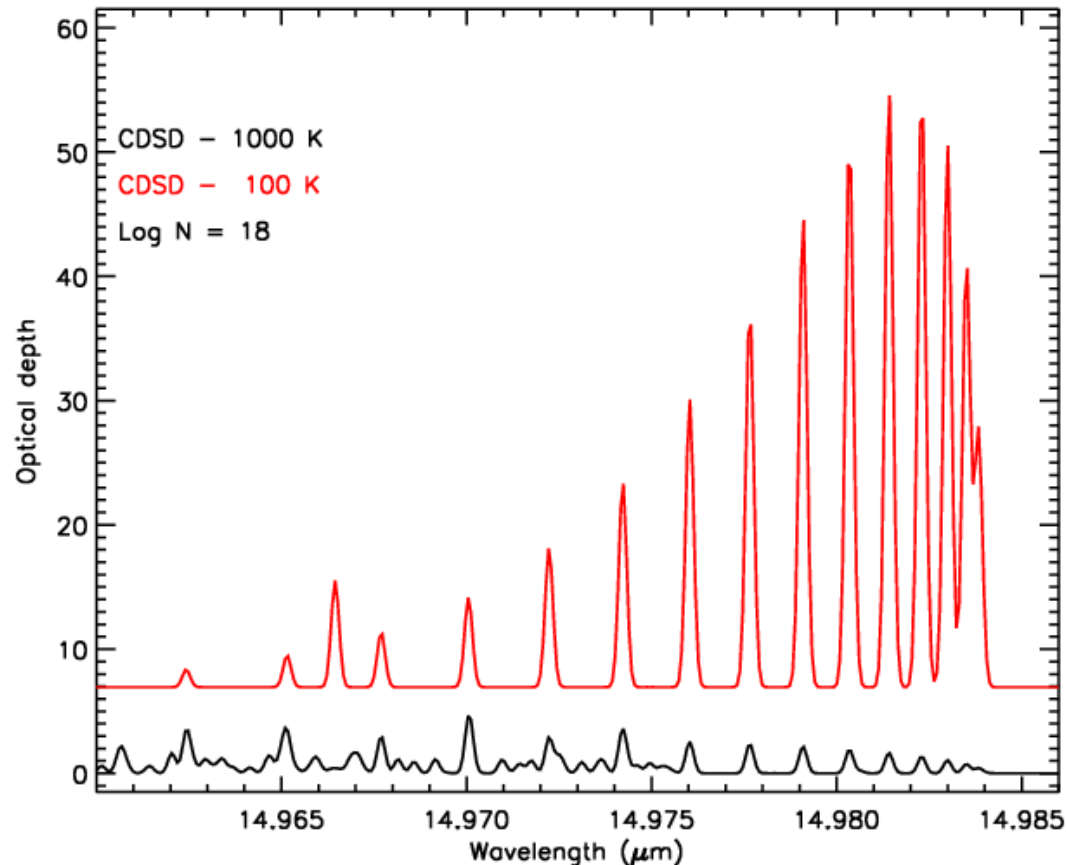
→ **Calculate line strength at desired T**



Model calculations II

Multiply line strength by column density
Convolve with intrinsic line profile

→ **Calculate optical depth**

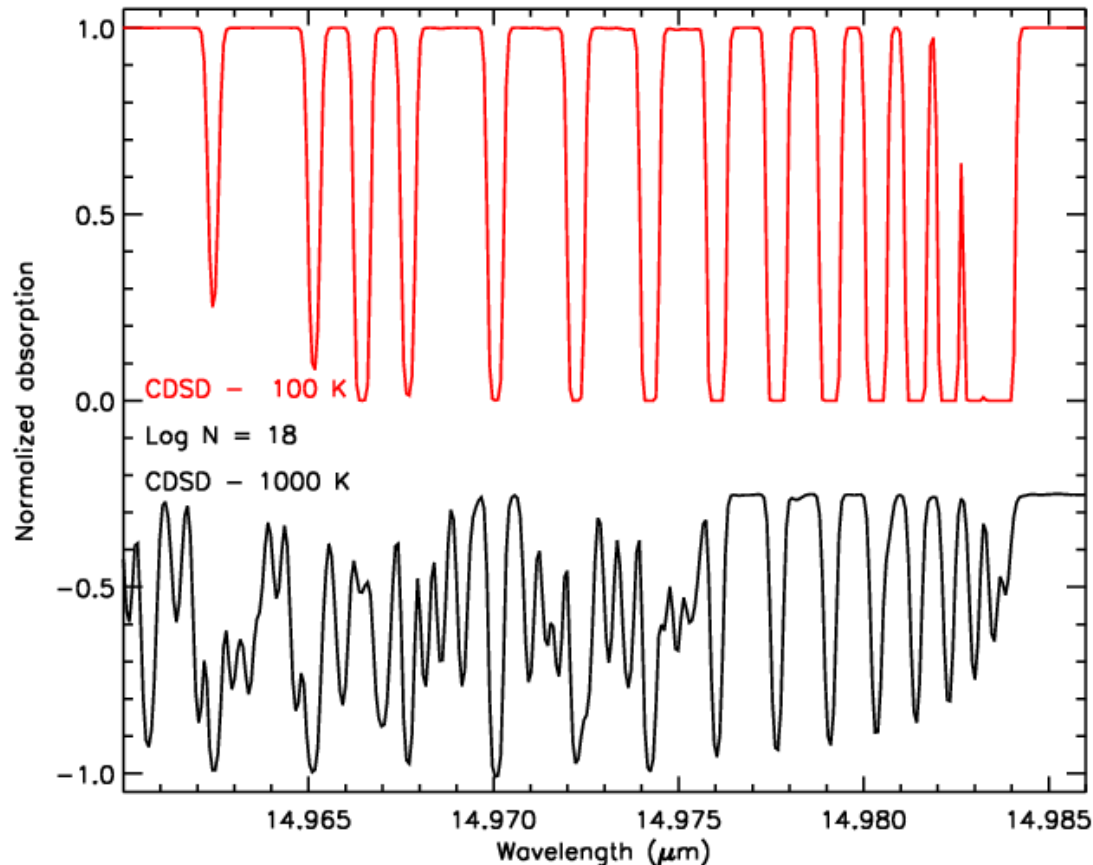


Model calculations III

Assume LTE & slab

How does this absorb radiation ?

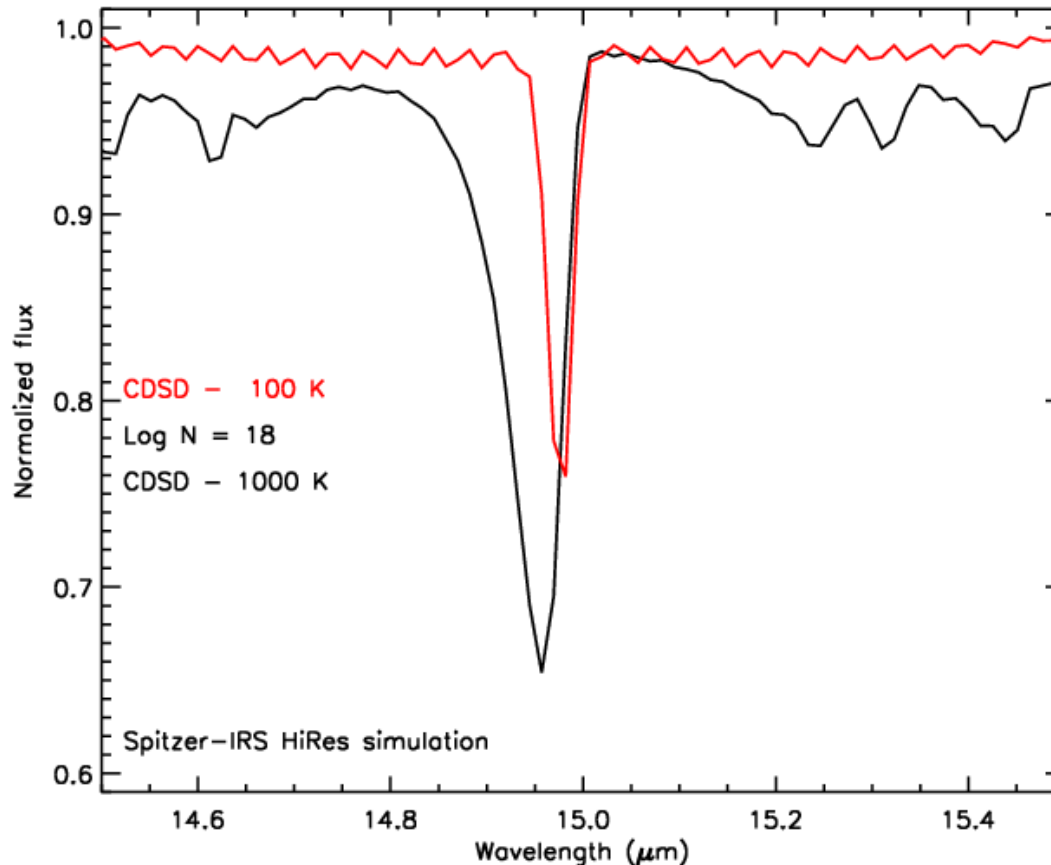
→ **Radiative transfer**



Model calculations IV

Convolve with instrument spectral response

→ Instrument simulation



Current contents of database

42 molecules (95 isotopologues)

25 different temperatures (100 K – 2500 K)

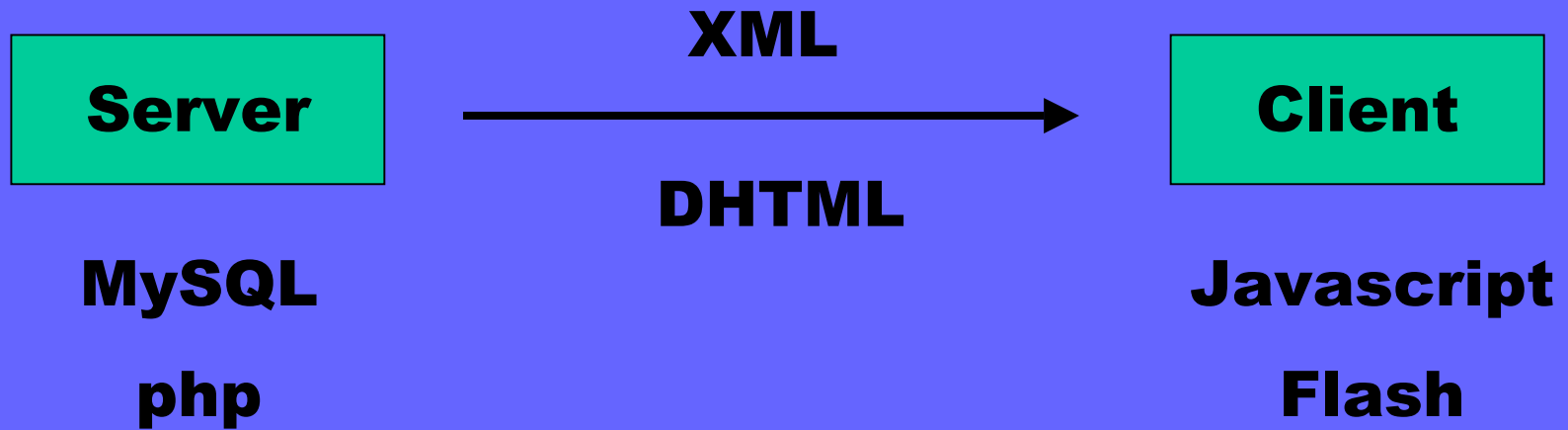
9 column densities (10^{16} – 10^{24} cm⁻²)

5 Instrument presets

291,213 model spectra (as of today)

Model spectra added by user requests !

The web interface - architecture



<http://www.spectrafactory.net/>

spectrafactory

A Database of 291213 Molecular Model Spectra - Cami & Markwick-Kemper, ApJS submitted.

NH₃, T=200.000, log(N)=22.400

(40 45224 1 01527)



Range Presets

Default

min

X

max

min Y max

1

100

0.0938748

1.0181225

Reset Zoom

Redisplay

Set as Default

browsespectra

Molecule K to K
 Isotopologue cm⁻² to cm⁻²
 Line List
 Instrument

searchresults

select count(*) from prv2 p where p.ml_id=1 and p.is_id=1 and temperature >= 500 and temperature <= 500 and log_columnndensity >= 18 and log_columnndensity <= 18

Found 15 spectra, showing 1 - 15

	Molecule	Isotopologue	Line List	T / K	log N / cm ⁻²	v / km s ⁻¹	Resolution	Oversample	Instrument
1	H ₂ O	H ₂ ¹⁶ O	Schwenke	500	18	3	2000	2	IRTF SpeX
2	H ₂ O	H ₂ ¹⁶ O	Schwenke	500	18	3	600	2	Spitzer-IRS HiRes 1
3	H ₂ O	H ₂ ¹⁶ O	HITEMP	500	18	3	120	2	Spitzer-IRS LowRes 2
4	H ₂ O	H ₂ ¹⁶ O	HITRAN04	500	18	3	120	2	Spitzer-IRS LowRes 2
5	H ₂ O	H ₂ ¹⁶ O	Schwenke	500	18	3	300	4	ISO-SWS AOT1, speed1
6	H ₂ O	H ₂ ¹⁶ O	Schwenke	500	18	3	120	2	Spitzer-IRS LowRes 2
7	H ₂ O	H ₂ ¹⁶ O	HITRAN04	500	18	3	2000	2	IRTF SpeX
8	H ₂ O	H ₂ ¹⁶ O	HITEMP	500	18	3	600	2	Spitzer-IRS HiRes 1
9	H ₂ O	H ₂ ¹⁶ O	HITRAN04	500	18	3	600	2	Spitzer-IRS HiRes 1
10	H ₂ O	H ₂ ¹⁶ O	HITEMP	500	18	3	90	2	Spitzer-IRS LowRes 1
11	H ₂ O	H ₂ ¹⁶ O	HITEMP	500	18	3	300	4	ISO-SWS AOT1, speed1
12	H ₂ O	H ₂ ¹⁶ O	Schwenke	500	18	3	90	2	Spitzer-IRS LowRes 1
13	H ₂ O	H ₂ ¹⁶ O	HITRAN04	500	18	3	300	4	ISO-SWS AOT1, speed1
14	H ₂ O	H ₂ ¹⁶ O	HITRAN04	500	18	3	90	2	Spitzer-IRS LowRes 1
15	H ₂ O	H ₂ ¹⁶ O	HITEMP	500	18	3	2000	2	IRTF SpeX

Found 15 spectra, showing 1 - 15

Needs & prospects

More / better line lists

Inaccurate line lists better than no line list

Theoretical calculations and/or laboratory work

Availability is only limit to our database !

Funding

This project is 0% funded

Observatories

Spitzer (now), soon SOFIA, Herschel, ALMA, ...

**143 molecules detected in space; many more
will be detected in the next years**